Acta Physica Hungarica 63(1–2), pp. 141–142 (1988)

A COMPUTER DATA ACQUISITION AND PROCESSING SYSTEM FOR RAMAN SPECTROSCOPY*

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(Received 15 September 1987)

A Varian Cary-82 laser Raman spectrometer was connected to a Nicolet 7199 FT-IR system. The Raman data acquisition system is based on a Commodore-128 microcomputer system. The software consists of two parts. The first one controls the data acquisition, the second one is a spectral data processing program. The new system has opened a series of new possibilities in vibrational spectroscopic research.

The increasing popularity and widening possibilities of the digital processing of spectral data have created a demand of connecting existing spectrometers with analogue data recording to computers. This was the aim of connecting our Varian Cary-82 laser Raman spectrometer to the Nicolet 1180 computer of a Nicolet 7199 FT-IR system [1]. The resulting system has all the benefits of the computer data acquisition and processing of Raman spectra [2], with the only disadvantage that for the time of Raman data acquisition, which may be as long as several hours, the 1180 computer is fully in use, and thus it cannot be used during this time for the control or processing of FT-IR measurements. Therefore, our new system has been developed in order to save time on the 1180 computer.

The new Raman data acquisition system is based on a Commodore-128, an 8-bit microcomputer. As peripherals, a Commodore 1571 floppy disk drive, a Commodore 1901 colour graphic display and an MPS 803 matrix printer are connected.

The microcomputer communicates with the Nicolet 1180 via a serial RS 232 C channel. The main peripherals of the latter computer are a Diablo 44 B hard disk drive and a Zeta digital plotter.

The spectrometer is connected to the microcomputer through two electronic units. The first one is a shaft encoder attached to the wavenumber drive of the Cary-82 spectrometer. Here, a disk with black and white sectors is fastened to a shaft which drives the mechanical wavenumber display wheels of the spectrometer, which gives, by means of opto-electric transducers, square pulses of a frequency proportional to the scan speed of the spectrometer. The second electronic unit is a counter interface. This counts, using a 24-bit synchronous counter, the amplified and shaped pulses arriving from the detector of the spectrometer (a photoelectron multiplier). The counter is controlled and the data are latched by the microcomputer through an INTEL 8255 A Programmable Parallel Peripheral Interface Processor.

The software of the microcomputer was written mostly in BASIC, but some functions

*Presented at the 3rd Hungarian Conference on Molecular Spectroscopy, Debrecen, Hungary, 24–28 August 1987 which were too slow or hard to perform in BASIC, were solved by means of ASSEMBLER routines written specially for this purpose.

According to basic functions, the software has been divided into two programs. The first one controls primarily data acquisition, which means mainly the control of the interface unit. Since the CPU time of the data input is relatively short (the input of 3 bytes at intervals of 0.2 to 10s), the peripheral interface processor requests an interrupt from the microcomputer when it is ready to send data. Then the CPU interrupts the execution of the running program and jumps to an interrupt service routine. The data are read by this routine. In the time between the interrupts the computer deals with display functions. In this manner, the progress of measurement can be seen continuously on the colour graphic display (in an arbitrary intensity and wavenumber scale, which may be changed interactively according to the intensity data of the spectrum).

Data acquisition stops automatically at a preset end frequency, it may be terminated, however, manually at any point. Thereafter, the spectrum and the main parameters of the measurement may be stored in a disk file with a name of up to 12 characters.

When developing the second program, for spectral data processing, it was taken into account that the Commodore microcomputer is able to communicate with the Nicolet 1180 computer through a serial RS 232 C channel, and that the software of the 1180 includes fast and user-friendly data processing routines. For this reason, and due to the relatively low speed of the Commodore, only the most important operations of data processing have been programmed on the Commodore microcomputer. These operations include, of course, the display of spectra and the determination of the frequency and intensity data of Raman bands by means of a graphic cursor. An important function of the program is spectrum accumulation, which can be used to improve the signal to noise ratio of the spectra by averaging, when other means for this (e.g. higher laser excitation energy) are not available.

The program also enables base line correction to be performed. This can be used to suppress fluorescence background which often hinders the evaluation of Raman spectra.

There are further data processing options provided by the software of Nicolet 1180:

By means of subtracting two spectra, it is possible to investigate the spectra of solutions in regions where the solvent has Raman band(s). This is equivalent to measurements on a "double beam" Raman spectrometer.

Curve analysis programs make it possible to determine the individual peak maxima and intensities of the components of overlapping band systems.

On the Zeta digital plotter connected to the Nicolet 1180 computer, high quality, optionally smoothed hard copies of the spectrum can be prepared, and any part of the spectrum can be expanded along either axes. It is possible to plot the infrared and Raman spectra of a compound in the same diagram, which is an aid in the assignment of vibrational bands to the normal modes of the molecule.

We feel that our computer controlled Raman data acquisition and processing system has opened new possibilities in theoretical and applied vibrational spectroscopic research.

References

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